(19)

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1621con

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
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NEWS 5	NOV 19	WPIX enhanced with XML display format
NEWS 6	NOV 30	ICSD reloaded with enhancements
NEWS 7	DEC 04	LINPADOCDB now available on STN
NEWS 8	DEC 14	BEILSTEIN pricing structure to change
NEWS 9	DEC 17	USPATOLD added to additional database clusters
NEWS 10	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 11	DEC 17	DGENE now includes more than 10 million sequences
NEWS 12	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 13	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 15	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 16	JAN 02	STN pricing information for 2008 now available
NEWS 17	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 18	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 19	JAN 28	MARPAT searching enhanced
NEWS 20	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 21	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23	FEB 08	STN Express, Version 8.3, now available
NEWS 24	FEB 20	PCI now available as a replacement to DPCI
NEWS 25	FEB 25	IFIREF reloaded with enhancements
NEWS 26	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 28	FEB 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 29	FEB 31	CAS REGISTRY enhanced with additional experimental spectra

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:16:56 ON 31 MAR 2008

=> FILE CSAREACT
'CSAREACT' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> FILE CASREACT

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'CASREACT' ENTERED AT 08:17:56 ON 31 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 29 Mar 2008 VOL 148 ISS 14

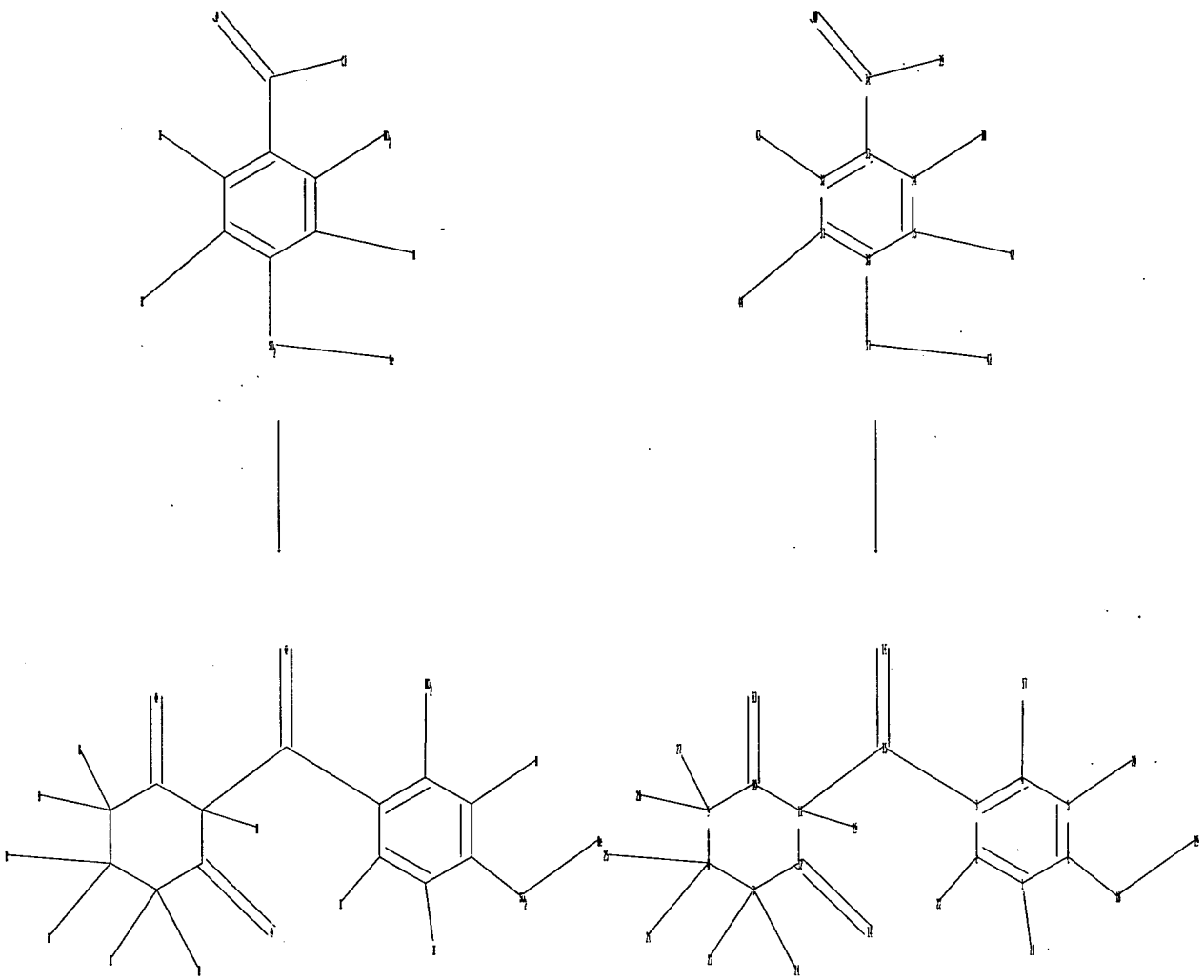
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 13.8 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\APP-102.str



chain nodes :
13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 36 37 38 39
40 41 42 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 30 31 32 33 34 35
chain bonds :
1-21 2-22 3-15 4-17 5-20 6-18 7-23 7-24 8-25 8-26 9-27 9-28 10-13
11-15 11-29 12-14 15-16 18-19 30-37 31-44 32-43 33-36 34-38 35-42 36-39
36-40 37-41
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 30-31 30-35
31-32 32-33 33-34 34-35
exact/norm bonds :
7-8 7-12 8-9 9-10 10-11 10-13 11-12 12-14 15-16 36-40
exact bonds :
1-21 2-22 3-15 4-17 5-20 6-18 7-23 7-24 8-25 8-26 9-27 9-28 11-15
11-29 18-19 30-37 31-44 32-43 33-36 34-38 35-42 36-39 37-41
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 30-31 30-35 31-32 32-33 33-34 34-35

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Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
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19:CLASS  20:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS
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44:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 30



L1      STRUCTURE UPLOADED

=> S L1 FULL
FULL SEARCH INITIATED 08:19:43 FILE 'CASREACT'
SCREENING COMPLETE -        2 REACTIONS TO VERIFY FROM        2 DOCUMENTS

100.0% DONE       2 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01

L2            0 SEA SSS FUL L1 (     0 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\APP-102.str product

L3      STRUCTURE UPLOADED

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Uploading C:\Program Files\Stnexp\Queries\APP-102.str reactant/reagent


=> S L3 FULL
FULL SEARCH INITIATED 08:20:42 FILE 'CASREACT'
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100.0% DONE      72 VERIFIED       3 HIT RXNS                    1 DOCS
SEARCH TIME: 00.00.01

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=> D L4 IBIB ABS CRD 1


L4   ANSWER 1 OF 1  CASREACT  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         131:31801  CASREACT
TITLE:                    Preparation of acylated cyclic 1,3-dicarbonyl
                          compounds by rearrangement of enol esters
INVENTOR(S):              Brown, Stephen Martin; Bentley, Thomas William; Jones,
                          Robert Oliver
PATENT ASSIGNEE(S):       Zeneca Limited, UK
SOURCE:                   PCT Int. Appl., 23 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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	RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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AU 9911671		A	19990616	AU 1999-11671	19981117
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EP 1034159		B1	20030122		
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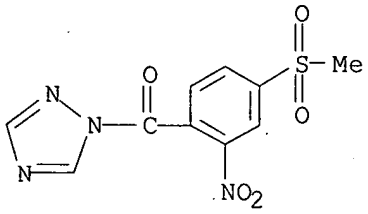
CN 1116266		B	20030730	CN 1998-809707	19981117
TW 528747		B	20030421	TW 1998-87119385	19981123
IN 191500		A1	20031206	IN 1998-DE3548	19981126
IL 134635		A	20050831	IL 1998-134635	19981127
US 6218579		B1	20010417	US 2000-529743	20000418
PRIORITY APPLN. INFO.:				GB 1997-25135	19971127
				WO 1998-GB3458	19981117

OTHER SOURCE(S): MARPAT 131:31801

GI For diagram(s), see printed CA Issue.

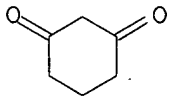
AB The title compds. [I; R = (un)substituted Ph, (un)substituted C3-6 cycloalkyl; Q = (un)substituted 5- or 6-membered saturated carbocyclic ring], especially benzoyl- and cycloalkyl-1,3-cyclohexanediones useful as herbicides and plant growth regulators (no data), were prepared by rearrangement of enol esters (II; Q, R as defined) in a (di)polar aprotic or aromatic hydrocarbon solvent in the presence of a moderate base and an azole instead of a cyanide catalyst. For example, stirring a mixture of 2.31 g 1,3-cyclohexanedione, 1.5 g K2CO3 and 20 mL MeCN for 3 h at 35°, adding 1.5 g PhCOCl and stirring for 30 min, adding 2 g K2CO3 and 0.035 g 1,2,4-triazole and stirring the whole for 16 h at 25° gave 2-benzoyl-1,3-cyclohexanedione in 90% yield.

RX(2) OF 10



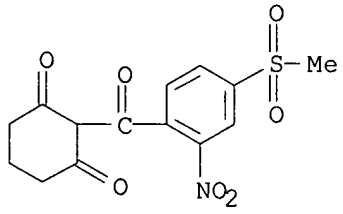
(step 1)

+



(step 1)

1. K2CO3, MeCN
2. HCl, Water



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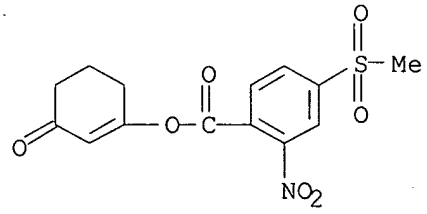
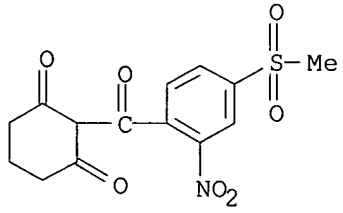
RX(6) OF 10



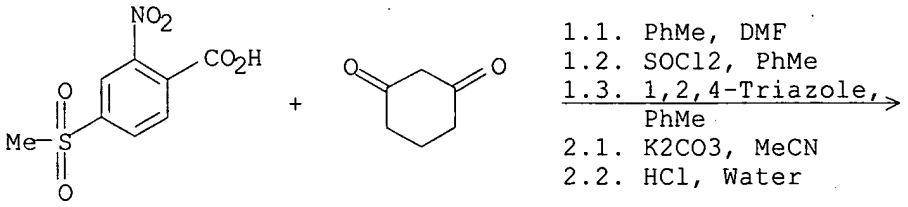
Bu4N.Br,
1,2,4-Triazole, K2CO3,
PhMe

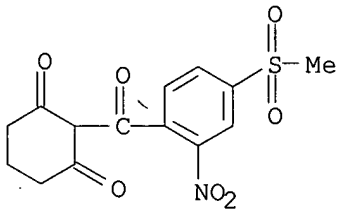


71%

NOTE: phase-transfer conditions are claimed

RX(10) OF 10 - 2 STEPS





100%

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	244.69	245.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

STN INTERNATIONAL LOGOFF AT 08:22:32 ON 31 MAR 2008

(2)

Connecting via Winsock to STN

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LOGINID:ssspta1621con

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 3	OCT 19	BEILSTEIN updated with new compounds
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NEWS 27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
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NEWS 29	FEB 31	CAS REGISTRY enhanced with additional experimental spectra

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:48:27 ON 31 MAR 2008

=> FILE CASREACT

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'CASREACT' ENTERED AT 08:49:49 ON 31 MAR 2008
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FILE CONTENT:1840 - 29 Mar 2008 VOL 148 ISS 14

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 13.8 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
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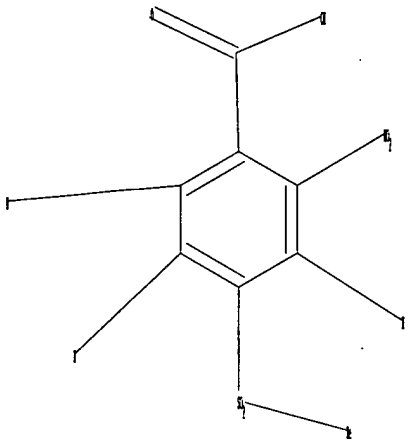

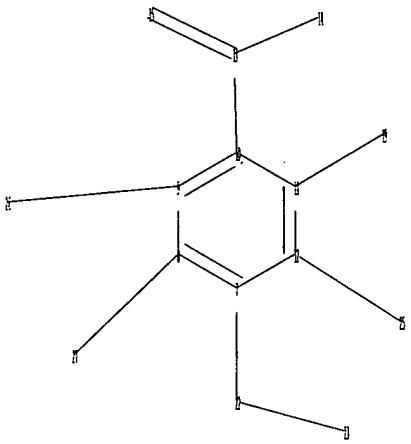

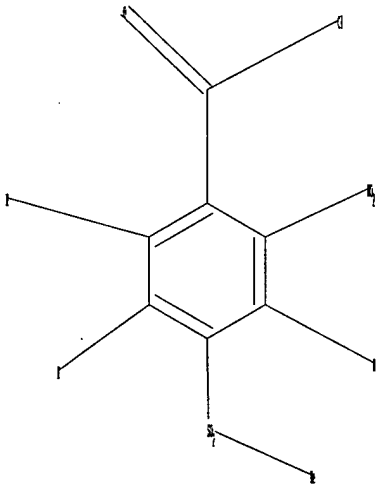

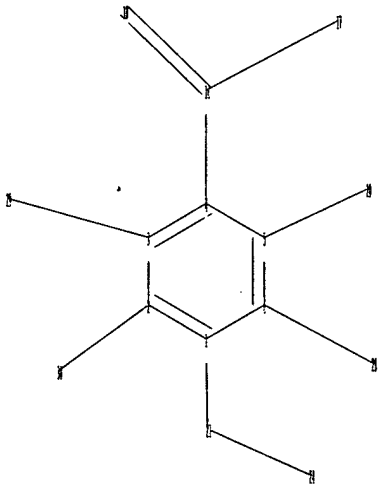

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ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-21 2-30 3-29 4-16 5-20 6-28 7-22 8-27 9-26 10-13 11-19 12-25 13-14
13-15 16-17 16-18 21-24 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
16-18
exact bonds :
1-21 2-30 3-29 4-16 5-20 6-28 7-22 8-27 9-26 10-13 11-19 12-25 16-17
21-24 22-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-15

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Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:CLASS  20:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS
27:CLASS  28:CLASS  29:CLASS  30:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7



L1      STRUCTURE UPLOADED

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SEARCH TIME: 00.00.01

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=>
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L3      STRUCTURE UPLOADED

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Uploading C:\Program Files\Stnexp\Queries\APP-121.str reactant/reagent

L4      STRUCTURE UPLOADED

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100.0% DONE      60 VERIFIED       9 HIT RXNS                       6 DOCS
SEARCH TIME: 00.00.01

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=> D L5 IBIB ABS CRD 1-6


L5   ANSWER 1 OF 6  CASREACT  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         144:88169  CASREACT
TITLE:                    Process for the preparation of substituted
                          bicyclooctenes and their use as herbicides
INVENTOR(S):              Beaudegnies, Renaud; Luethy, Christoph; Edmunds,
                          Andrew; Schaetzer, Juergen; Wendeborn, Sebastian
PATENT ASSIGNEE(S):       Syngenta Participations AG, Switz.
SOURCE:                   PCT Int. Appl., 109 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: CH 2004-1050 20040622
CH 2004-1051 20040622

OTHER SOURCE(S): MARPAT 144:88169

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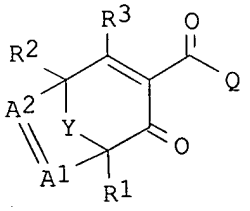

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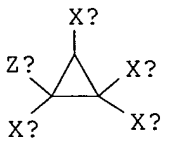
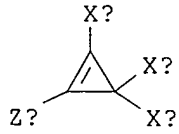
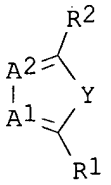


II



III

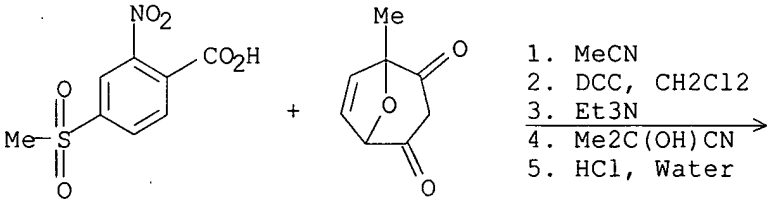


IV

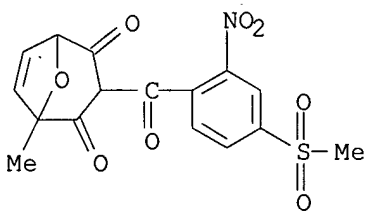
AB Compds. I [A1 = N, CR7, A2 = N, CR8; R1, R2, R7, R8 = H, C1-6-alkyl, C2-6-alkenyl, C2-6-alkynyl, halogen, OH, SH, NO2, CN, (C1-6-alkoxy)carbonyl, (C1-6-alkyl)carbonyl, CHO, CH:NOH, (C1-6-alkoxy)iminomethylene, C1-6-alkoxy, C1-6-haloalkoxy, C3-6-alkenyloxy, C3-6-alkynyloxy, (C1-4-alkoxy)-(C1-2-alkoxy), (C1-6-alkoxy)carbonyloxy, C1-6-alkylthio, C1-6-alkylsulfonyl, C1-6-alkylsulfinyl, etc.; R3 = OH, O-M+, halogen, C1-8-alkoxy, SH, C1-8-alkylthio, C1-8-alkylsulfinyl, C1-8-alkylsulfonyl, C1-8-haloalkylthio, C1-8-haloalkylsulfinyl, C1-8-haloalkylsulfonyl, (C1-4-alkoxy)-(C1-4-alkyl)thio, (C1-4-alkoxy)-(C1-4-alkyl)sulfinyl, (C1-4-alkoxy)-(C1-4-alkyl)sulfonyl, (C3-8-alkenyl)thio, (C3-8-alkynyl)thio, (C1-4-alkylthio)-(C1-4-alkyl)thio, (C3-4-alkenyl)thio-(C1-4-alkyl)thio, (C1-4-alkoxy)carbonyl-(C1-4-alkyl)thio, (C1-4-alkoxy)carbonyl-(C1-4-alkyl)sulfinyl, (C1-4-alkoxy)carbonyl-(C1-4-alkyl)sulfonyl, etc.; M+ = alkali metal ion, ammonium cation; Q = Ph (optionally substituted with up to 4 substituents); Y = O, NR4a, S, S(:O), SO2, C(:O), C(:NR4b), C(:CR6aR6b), C1-4-alkylene, C2-4-alkenylene; R4a = ; R4b = ; R6a = H, C1-6-alkyl, (C1-6-alkyl)carbonyl, (C1-6-alkyl)carbonyloxy; R6b = H, C1-6-alkyl; R6aR6b = C2-5-alkylene] are suitable for use as herbicides. The process for the preparation of substituted bicyclooctenes comprises: (a) converting cyclopropane II [Xa = H, Cl, Br, I; Xb, Xc, Xd = halogen; Za = halogen, C1-6-alkoxy, OPh, C1-6-alkylthio, C1-6-alkylsulfinyl, C1-6-alkylsulfonyl, SPh, S(:O)Ph, SO2Ph] in an anhydrous inert solvent containing an alkali metal hydroxide to cyclopropene III; (b) reacting III with cyclopentadiene IV; and (c) hydrolysis in the presence of an aqueous base. Thus, 3-[4-(Methanesulfonyl)-2-nitrobenzoyl]bicyclo[3.2.1]oct-6-ene-2,4-dione [I; A1 = A2 = CH, Q = C6H4NO2-2-(SO2Me)-4, R1 = R2 = H, R3 = OH, Y = CH2] was prepared from cyclopentadiene via cycloaddn. with

pentachlorocyclopropane in dioxane containing KOH, hydrolysis with aqueous NaOH,
reduction with Zn in AcOH, and acylation with 4-(methanesulfonyl)-2-nitrobenzoic acid in MeCN containing dicyclohexylcarbodiimide in CH2Cl2, Et3N and acetone cyanohydrin. The pre- and post-emergence herbicidal activity of I [A1 = A2 = CH, Q = C6H4NO2-2-(SO2Me)-4, R1 = R2 = H, R3 = OH, Y = CH2; (at 250 g/ha)] was determined [pre-emergence: total damage = 9/10 vs. Panicum; total damage = 9/10 vs. Echinochloa; total damage = 9/10 vs. Amaranthus; total damage = 9/10 vs. Sinapis; total damage = 9/10 vs. Stellaria; post-emergence: total damage = 7/10 vs. Echinochloa; total damage = /10 vs. Xanthium; total damage = 9/10 vs. Ipomea; total damage = 10/10 vs. Chenopodium; total damage = 9/10 vs. Kochia; total damage = 9/10 vs. Sinapis; total damage = 9/10 vs. Stellaria].

RX(19) OF 34



(step 1) (step 1)



CON: STAGE(1) room temperature
STAGE(2) 2.5 hours, room temperature
STAGE(3) room temperature
STAGE(4) 18 hours, room temperature
STAGE(5) room temperature, pH 1

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 6 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:459878 CASREACT
TITLE: Multi-step process for the production of cyclic diketones
INVENTOR(S): Jackson, David Anthony; Edmunds, Andrew; Bowden, Martin Charles; Brockbank, Ben
PATENT ASSIGNEE(S): Syngenta Participations AG, Switz.; Syngenta Limited
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105745	A1	20051110	WO 2005-EP4681	20050429

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,

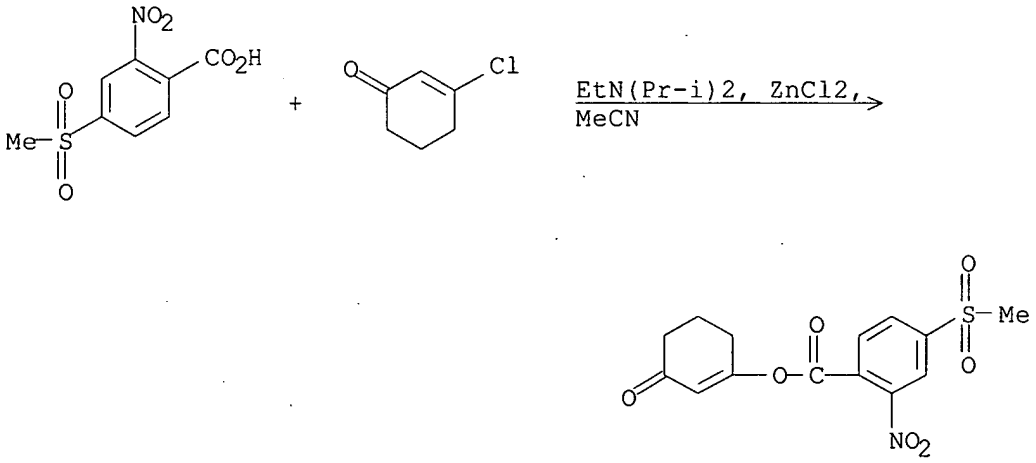
NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005238195	A1	20051110	AU 2005-238195	20050429
EP 1756059	A1	20070228	EP 2005-741812	20050429
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1950339	A	20070418	CN 2005-80013706	20050429
BR 2005010502	A	20071030	BR 2005-10502	20050429
JP 2007535516	T	20071206	JP 2007-509989	20050429
US 20070232837	A1	20071004	US 2006-568337	20061026
IN 2006CN04011	A	20070810	IN 2006-CN4011	20061101
PRIORITY APPLN. INFO.:			CH 2004-765	20040430
			WO 2005-EP4681	20050429

OTHER SOURCE(S): MARPAT 143:459878

AB A multi-step process for the preparation of cyclic diketones [e.g., 4-(4-chlorophenylcarbonyloxy)bicyclo[3.2.1]oct-3-en-2-one] is presented.

RX(10) OF 15



CON: STAGE(1) 15 minutes, room temperature; 18 hours, 45 deg C; 45 deg C -> reflux; 40 hours, reflux

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	143:459877 CASREACT
TITLE:	Process for the production of cyclic diketones
INVENTOR(S):	Jackson, David Anthony; Edmunds, Andrew; Bowden, Martin Charles; Brockbank, Ben
PATENT ASSIGNEE(S):	Syngenta Participations A.-G., Switz.; Syngenta Limited
SOURCE:	PCT Int. Appl., 28 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105718	A2	20051110	WO 2005-EP4680	20050429
WO 2005105718	A3	20060504		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005238194	A1	20051110	AU 2005-238194	20050429
CA 2562152	A1	20051110	CA 2005-2562152	20050429
EP 1740524	A2	20070110	EP 2005-738471	20050429

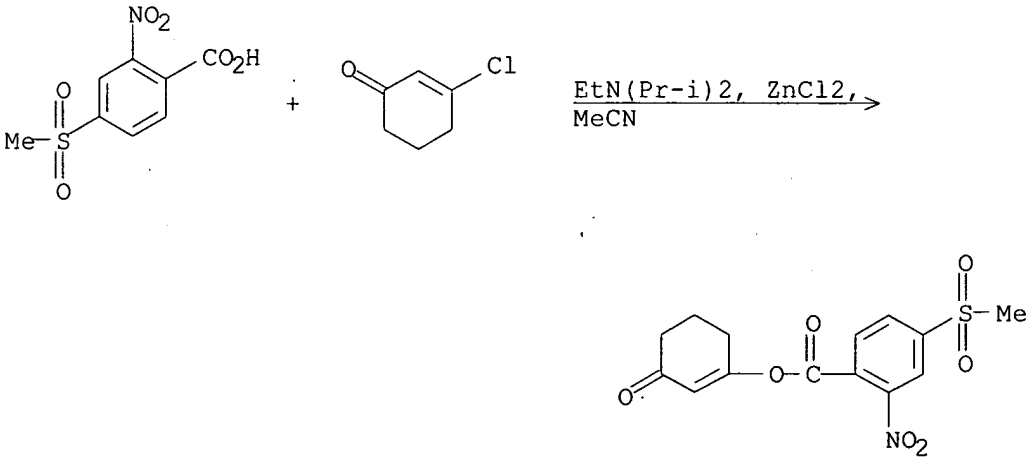
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

CN 1950319	A	20070418	CN 2005-80013809	20050429
BR 2005010492	A	20071113	BR 2005-10492	20050429
JP 2007535515	T	20071206	JP 2007-509988	20050429
MX 2006PA12161	A	20070117	MX 2006-PA12161	20061020
KR 2007008671	A	20070117	KR 2006-722687	20061030
IN 2006CN04021	A	20070810	IN 2006-CN4021	20061101
PRIORITY APPLN. INFO.:			CH 2004-766	20040430
			WO 2005-EP4680	20050429

OTHER SOURCE(S): MARPAT 143:459877

AB A process for the preparation of cyclic diketones [e.g., 4-(4-chlorophenylcarbonyloxy)bicyclo[3.2.1]oct-3-en-2-one] is presented.

RX(3) OF 12



CON: STAGE(1) 15 minutes, room temperature;
room temperature -> 45 deg C; 18 hours, 45 deg C;
45 deg C -> reflux; 40 hours, reflux

L5 ANSWER 4 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

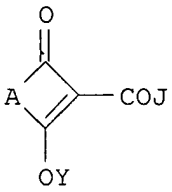
ACCESSION NUMBER:	140:42165 CASREACT
TITLE:	Acylation of cyclic 1,3-diketones with Ph esters in the presence of cyanide or fluoride ion.
INVENTOR(S):	Wojtkowski, Paul Walter

PATENT ASSIGNEE(S): E.I. Du Pont de Nemours and Co., USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp., Cont.-in-part of U.S. Ser. No. 833,451, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030232984	A1	20031218	US 2003-396047	20030324
US 6809206	B2	20041026		
US 20020049317	A1	20020425	US 2001-833451	20010412

PRIORITY APPLN. INFO.: US 1999-120213P 19990212
US 2000-483644 20000114
US 2001-833451 20010412

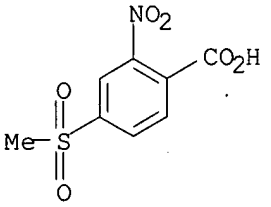
OTHER SOURCE(S): MARPAT 140:42165
GI



I

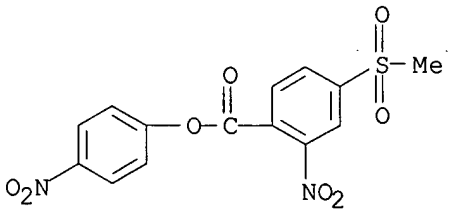
AB Title compds. [I; A = linker comprising 2-4 C, 0-2 N, 0-2 O, and 0-2 S atoms; J = (substituted) C-linked hydrocarbyl; Y = H, salt cation], were prepared by treatment of the corresponding diketones with RyC6H5-yO2CJ (R = electron withdrawing group; y = 0-3; J as above) in the presence of CN- or F-. Thus, 2-(methoxycarbonyl)phenyl 2,3-dihydro-5,8-dimethylspiro(4H-1-benzothiopyran-4,2'-[1,3]dioxolane)-6-carboxylate 1,1-dioxide (preparation given), 1,3-cyclohexanedione, Et3N, and KCN were heated in MeCN in a sealed tube for 10 h at 90° to give 2-[[2,3-dihydro-5,8-dimethyl-1,1-dioxidospiro(4H-1-benzothiopyran-4,2'-[1,3]dioxolan)-6-yl]carbonyl]-3-hydroxy-2-cyclohexen-1-one Et3N salt.

RX(25) OF 31



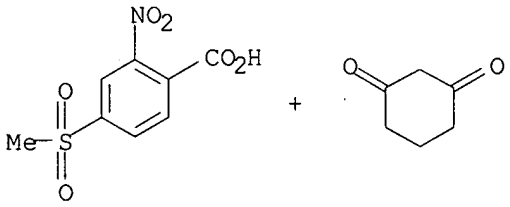
1. DMF, (COCl)2, CH2Cl2
2. 4-O2NC6H4OH, Et3N, CH2Cl2

(step 1)

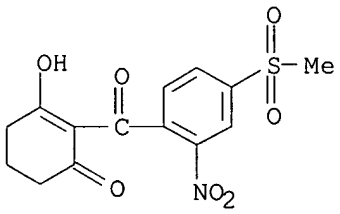


CON: STAGE(1) room temperature; 1 hour, room temperature
STAGE(2) room temperature; 1 hour, room temperature

RX(30) OF 31 - 2 STEPS



1.1. DMF, (COCl)2, CH2Cl2
1.2. 4-O2NC6H4OH, Et3N, CH2Cl2
2.1. Me2C(OH)CN, Et3N, MeCN
2.2. NaHCO3, Water



CON: STEP(1.1) room temperature; 1 hour, room temperature
STEP(1.2) room temperature; 1 hour, room temperature
STEP(2) 1 hour, 22 deg C

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

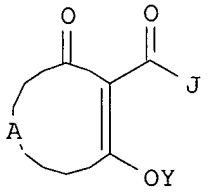
L5 ANSWER 5 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	136:340425 CASREACT
TITLE:	Method for acylating cyclic 1,3-diketones with phenyl ester derivatives to yield triketones
INVENTOR(S):	Wojtkowski, Paul Walter
PATENT ASSIGNEE(S):	USA
SOURCE:	U.S. Pat. Appl. Publ., 20 pp., Cont.-in-part of U. S. Ser. No. 483,644. CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

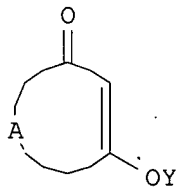
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020049317	A1	20020425	US 2001-833451	20010412
US 20030232984	A1	20031218	US 2003-396047	20030324
US 6809206	B2	20041026		
PRIORITY APPLN. INFO.:			US 2000-483644	20000114
			US 1999-120213P	19990212
			US 2001-833451	20010412

OTHER SOURCE(S): MARPAT 136:340425

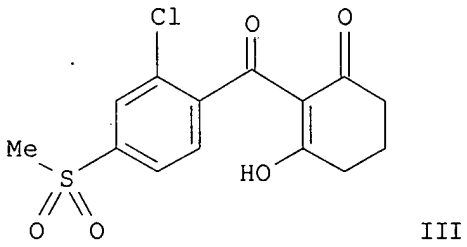
GI



I



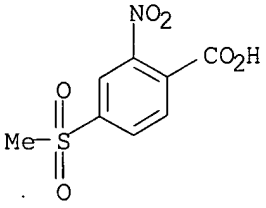
II



III

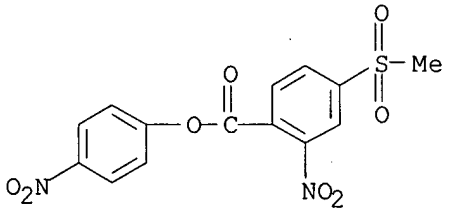
AB A method is disclosed for the preparation of I by acylation of II with Ar-OCOJ in the presence of a cyanide or fluoride catalyst [A = linking group comprising an (un)substituted backbone segment consisting of 2 to 4 atoms selected from carbon atoms and 0-2 N, O, or S atoms; J = (un)substituted, carbon-linked hydrocarbyl group; Y = H or a salt cation; Ar = (un)substituted phenyl]. Forty-one examples are provided. For instance, 2-[2-chloro-4-(methylsulfonyl)benzoyl]-3-hydroxy-2-cyclohexen-1-one (III) was prepared from 4-nitrophenyl 2-chloro-4-(methylsulfonyl)benzoate (preparation given) and 1,3-cyclohexanedione in the presence of acetone cyanohydrin and triethylamine in acetonitrile for 3 h at 22°C. Ph ester substitution and sources of cyanide and fluoride were evaluated in the examples. Utilization of Ph esters as acylation agents worked well in the one step process and can be prepared under mild, acid-free conditions preserving sensitive functionality vulnerable to degradation under reaction conditions used to prepare acyl chlorides of prior art processes.

RX(23) OF 28

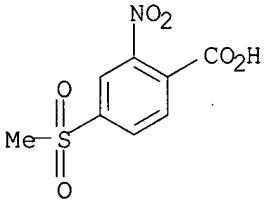


(step 1)

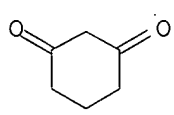
1. (COCl)2, CH2Cl2
2. 4-O2NC6H4OH, Et3N



RX(27) OF 28 - 2 STEPS

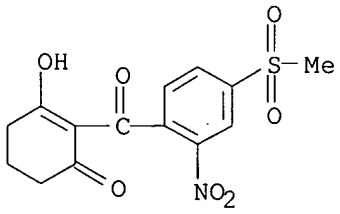


+



(step 2)

1.1. (COCl)2, CH2Cl2
1.2. 4-O2NC6H4OH, Et3N
2. Me2C(OH)CN, Et3N, MeCN



L5 ANSWER 6 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 131:31801 CASREACT
TITLE: Preparation of acylated cyclic 1,3-dicarbonyl compounds by rearrangement of enol esters
INVENTOR(S): Brown, Stephen Martin; Bentley, Thomas William; Jones, Robert Oliver
PATENT ASSIGNEE(S): Zeneca Limited, UK
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9928282	A1	19990610	WO 1998-GB3458	19981117

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,

NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

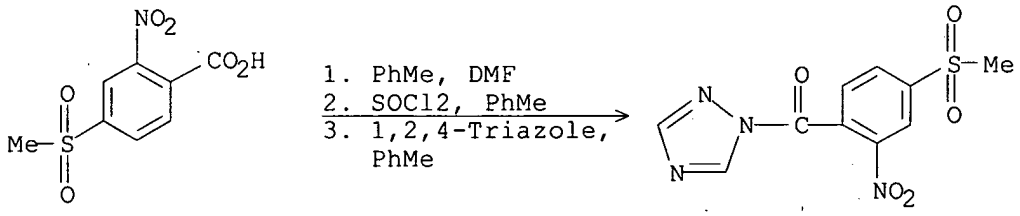
CA 2295892	A1	19990610	CA 1998-2295892	19981117	
CA 2295892	C	20080205			
AU 9911671	A	19990616	AU 1999-11671	19981117	
EP 1034159	A1	20000913	EP 1998-954618	19981117	
EP 1034159	B1	20030122			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
BR 9815026	A	20001003	BR 1998-15026	19981117	
HU 2000004664	A2	20010528	HU 2000-4664	19981117	
JP 2001524539	T	20011204	JP 2000-523183	19981117	
AT 231483	T	20030215	AT 1998-954618	19981117	
ES 2187073	T3	20030516	ES 1998-954618	19981117	
PT 1034159	T	20030630	PT 1998-954618	19981117	
CN 1116266	B	20030730	CN 1998-809707	19981117	
TW 528747	B	20030421	TW 1998-87119385	19981123	
IN 191500	A1	20031206	IN 1998-DE3548	19981126	
IL 134635	A	20050831	IL 1998-134635	19981127	
US 6218579	B1	20010417	US 2000-529743	20000418	
PRIORITY APPLN. INFO.:			GB 1997-25135	19971127	
			WO 1998-GB3458	19981117	

OTHER SOURCE(S): MARPAT 131:31801

GI For diagram(s), see printed CA Issue.

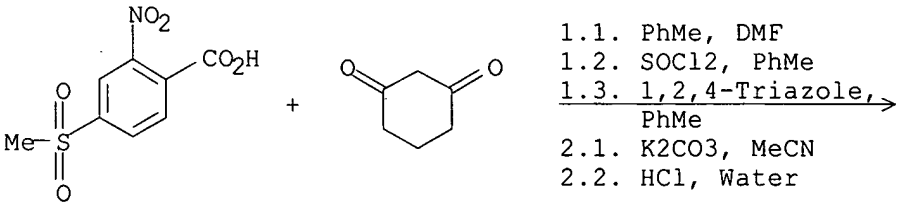
AB The title compds. [I; R = (un)substituted Ph, (un)substituted C3-6 cycloalkyl; Q = (un)substituted 5- or 6-membered saturated carbocyclic ring], especially benzoyl- and cycloalkyl-1,3-cyclohexanediones useful as herbicides and plant growth regulators (no data), were prepared by rearrangement of enol esters (II; Q, R as defined) in a (di)polar aprotic or aromatic hydrocarbon solvent in the presence of a moderate base and an azole instead of a cyanide catalyst. For example, stirring a mixture of 2.31 g 1,3-cyclohexanedione, 1.5 g K2CO3 and 20 mL MeCN for 3 h at 35°, adding 1.5 g PhCOCl and stirring for 30 min, adding 2 g K2CO3 and 0.035 g 1,2,4-triazole and stirring the whole for 16 h at 25° gave 2-benzoyl-1,3-cyclohexanedione in 90% yield.

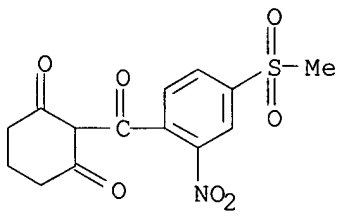
RX(8) OF 10



(step 1) 57%

RX(10) OF 10 - 2 STEPS





100%

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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---Logging off of STN---

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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